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DEVELOPMENT OF SHARP DISCONTINUITY TRACKING METHODS FOR EXPLOSION PROBLEMS

BY GREGORY R. SHUBIN

RESEARCH AND TECHNOLOGY DEPARTMENT

3 NOVEMBER 1978

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This report summarizes the development of a new numerical method called "sharp discontinuity tracking" for predicting the flow field arising in explosive blast problems. This method uses standard finite difference techniques for smooth regions of the flow, but treats physically important shocks and contact discontinuities as explicit surfaces (internal boundaries) which remain "sharp" (not smeared) as the computation progresses. The method

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SUMMARY

This report describes a computational method called "sharp discontinuity tracking" which is a new approach for accurately predicting the flow field arising in explosion problems. This work was performed by the author who is a member of the Applied Mathematics Branch of NSWC. The guidance and advice of Dr. Jay Solomon of NSWC was invaluable and is gratefully acknowledged.

Paul R. Wessel

PAUL R. WESSEL
By direction

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ILLUSTRATIONS

1. INTRODUCTION

Many problems of interest involve the propagation of blast waves arising from explosions, and the interaction of these waves with boundaries. In principle, a computational solution of this fluid dynamics problem should provide a cost-effective alternative to expensive physical experimentation. In reality, the computational problem is an extremely difficult one which involves the propagation and interaction of various discontinuities, both shock waves and contact discontinuities (e.g., interfaces between different materials), in more than one space dimension. It is of practical interest to get accurate results for the shock pressure profile (especially the peak pressure) and also to correctly predict the motion of material interfaces which significantly affect the flow field.

Finite difference methods currently in use (both Lagrangian and Eulerian) for these explosion problems use either explicit or implicit artificial viscosity to spread or smear shocks over several computational mesh points. This falsifies the peak shock pressure and impulse. To obtain sufficient accuracy, it is necessary to use a very large number of mesh points, which becomes prohibitive for complicated multidimensional problems. While pure Lagrangian methods can follow material interfaces well and can allow areas of fine resolution to move with the fluid, they ultimately tend to break down because severe material deformation leads to distorted computational meshes. Pure Eulerian methods can handle distortion and internal slip but produce diffusion of material interfaces and do not readily allow localized resolution.

This research is aimed at developing a new numerical method called "sharp discontinuity tracking" which will follow shocks and contact discontinuities accurately without introducing smearing or computational oscillations. While the method is specifically designed to handle the problem of determining the pressure history under water due to a chemical <u>e</u>xplosion in <u>a</u>ir <u>a</u>bove a <u>w</u>ater surface (herein called the "EAAW problem"), it should be applicable to other explosion dynamics problems of interest. This method allows for adequate computational resolution of physically small or shrinking regions which contain important physical phenomena, such as the air region between the expanding explosive gases and the water surface in the EAAW problem just described.

The present method is based partly on the work of Solomon et al. [References 1,2] who developed a computational method for predicting the three-dimensional steady supersonic flow field over reentry vehicles at angles of attack. Since such a steady flow problem is hyperbolic with the axial direction being a time-like coordinate, it is similar to the two-dimensional axisymmetric unsteady flow case considered here.

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1. Solomon, J. M., et al., "A Program for Computing Steady Inviscid Three-Dimensional Supersonic Flow on Reentry Vehicles, Vol I: Analysis and Programming," NSWC/WOL TR 77-28, 11 Feb 1977.
2. Solomon, J. M., et al., "Inviscid Flowfield Calculations for Reentry Vehicles with Control Surfaces," <u>AIAA Journal</u>, Vol. 15, No. 12, Dec 1977, p. 1742.

2. OVERVIEW OF COMPUTATIONAL METHOD

A. GENERAL DESCRIPTION OF METHOD. The method of sharp discontinuity tracking is a finite difference method for obtaining approximate solutions of the nonlinear system of hyperbolic conservation laws (partial differential equations) which describe inviscid fluid dynamics. The proposed methodology is schematically indicated in Figure 1. It is distinct from the usual finite difference methods since it defines explicit surfaces in the computational field which represent physical discontinuities, both shock waves and contact discontinuities. A special system of finite difference equations governs the motion of these surfaces and exactly enforces the physical boundary conditions which must hold across the discontinuities. No finite differences are taken across these surfaces. Since the discontinuities are perfectly sharp, interactions can be treated by locally exact methods.

In practice it proves useful to perform a time-dependent coordinate transformation to obtain a regular mesh in which the contact surfaces are always coordinate lines and the shocks "float" through the Eulerian mesh. The regions of relatively smooth flow between the discontinuities can be accurately handled by standard second order accurate finite difference methods.

A much more detailed description of the method is given in Appendix A.

B. TRACKING OF DISCONTINUITIES. The surfaces of discontinuity represent physical shock waves and contact discontinuities. The motion of these surfaces is determined by the physical conditions which must hold across the surfaces and is also influenced by the surrounding fluids. The correct conditions linking the values of flow variables on either side of the surfaces are the Rankine-Hugoniot jump conditions for a shock, and the equality of pressure and normal particle velocity for a contact discontinuity. The surrounding fluid can influence the surface only in certain ways determined by the theory of characteristics for a system of hyperbolic partial differential equations. By selecting appropriate admissible characteristic compatability relations and combining them with the correct physical boundary conditions, one obtains a system of differential equations which governs the motion of the surface and gives the flow variables on either side as a function of time. These differential equations are then discretized to give a system of finite difference equations for advancing the discontinuity in time.

C. INTERACTION OF DISCONTINUITIES. The surfaces of discontinuity move relative to each other and will in general collide and interact. Where they meet they are locally plane and the values of flow variables on either side are explicitly known. The interaction then reduces to an algebraic problem of finding a configuration of transmitted and reflected discontinuities which satisfy all of the necessary conditions in the infinitesimal neighborhood surrounding the point of intersection. This locally exact solution is explicitly inserted into the computed flow field.

D. EXPECTED ADVANTAGES OF METHOD.

(i) Greater accuracy for individual discontinuities since they remain perfectly sharp (not smeared). Hence more accurate peak shock pressures and impulses.

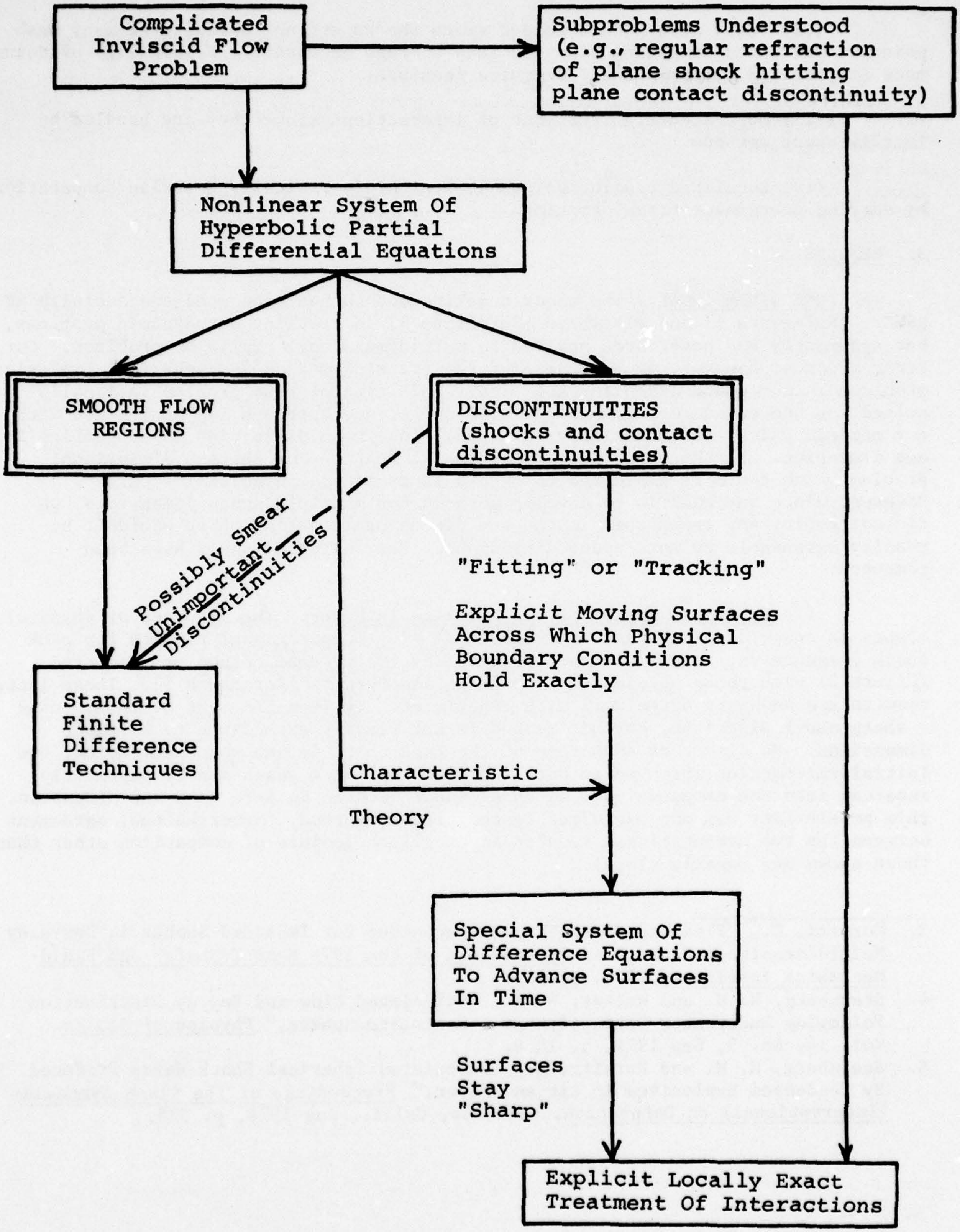

FIGURE 1 OVERVIEW OF COMPUTATIONAL METHODOLOGY

(ii) Fewer mesh points needed since shocks are not spread over many mesh points. Decreased computing time and less storage necessary. Possibility of doing more complicated problems than otherwise feasible.

(iii) More accurate treatment of interactions since they are handled by locally exact methods.

(iv) Localized resolution possible within a basically Eulerian computation by varying coordinate transformation.

3. RESULTS

A. ONE DIMENSIONAL. The shock tracking method has been used successfully at NSWC [Reference 1] and elsewhere [Reference 3] in treating aerodynamic problems, but apparently has never been applied to multidimensional explosion problems. Our first efforts, however, were to develop the tracking method for spherical explosion problems in one space dimension and time. This type of test problem is ideally suited for the standard Lagrangian finite difference approach (as contrasted with our methods which are essentially Eulerian) since mesh distortion is no problem in one dimension. Furthermore, there are special features of the one dimensional problem which could be exploited to obtain increased computational accuracy. However, since our goal is to develop methods for multiple space dimensions, we did not employ any techniques in the one dimensional testing which wouldn't be readily extendable to more space dimensions. The following cases have been computed:

(i) Spherical Explosion of Pentolite in Water. The sequence of physical events is described in detail in [Reference 4]. Computational results for peak shock pressure vs. radial distance obtained by the present method are compared (Figure 2) with those obtained by Sternberg and Hurwitz [Reference 5]. These latter results are known to agree well with experiment. It is noted that Sternberg used a sharp shock algorithm, but his method is not readily extendable to multiple dimensions. He also took advantage of the fact that, in one space dimension, the initial rarefaction which moves back into the explosive gases can be explicitly inserted into the computation. As this cannot be done in more than one dimension, this possibility was not exploited by the present method. Nevertheless, agreement between the two computational results is excellent (points of comparison other than those shown are equally close).

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3. Moretti, G., "Floating Shock Fitting Technique for Imbedded Shocks in Unsteady Multidimensional Flows," in Proceedings of the 1974 Heat Transfer and Fluid Mechanics Institute, 1974, p. 184.
4. Sternberg, H. M. and Walker, W. A., "Calculated Flow and Energy Distribution Following Underwater Detonation of a Pentolite Sphere," Physics of Fluids, Vol. 14, No. 9, Sep 1971, p. 1869.
5. Sternberg, H. M. and Hurwitz, H., "Calculated Spherical Shock Waves Produced By Condensed Explosives in Air and Water," Proceedings of the Sixth Symposium (International) on Detonation, Coronado, Calif., Aug 1976, p. 528.

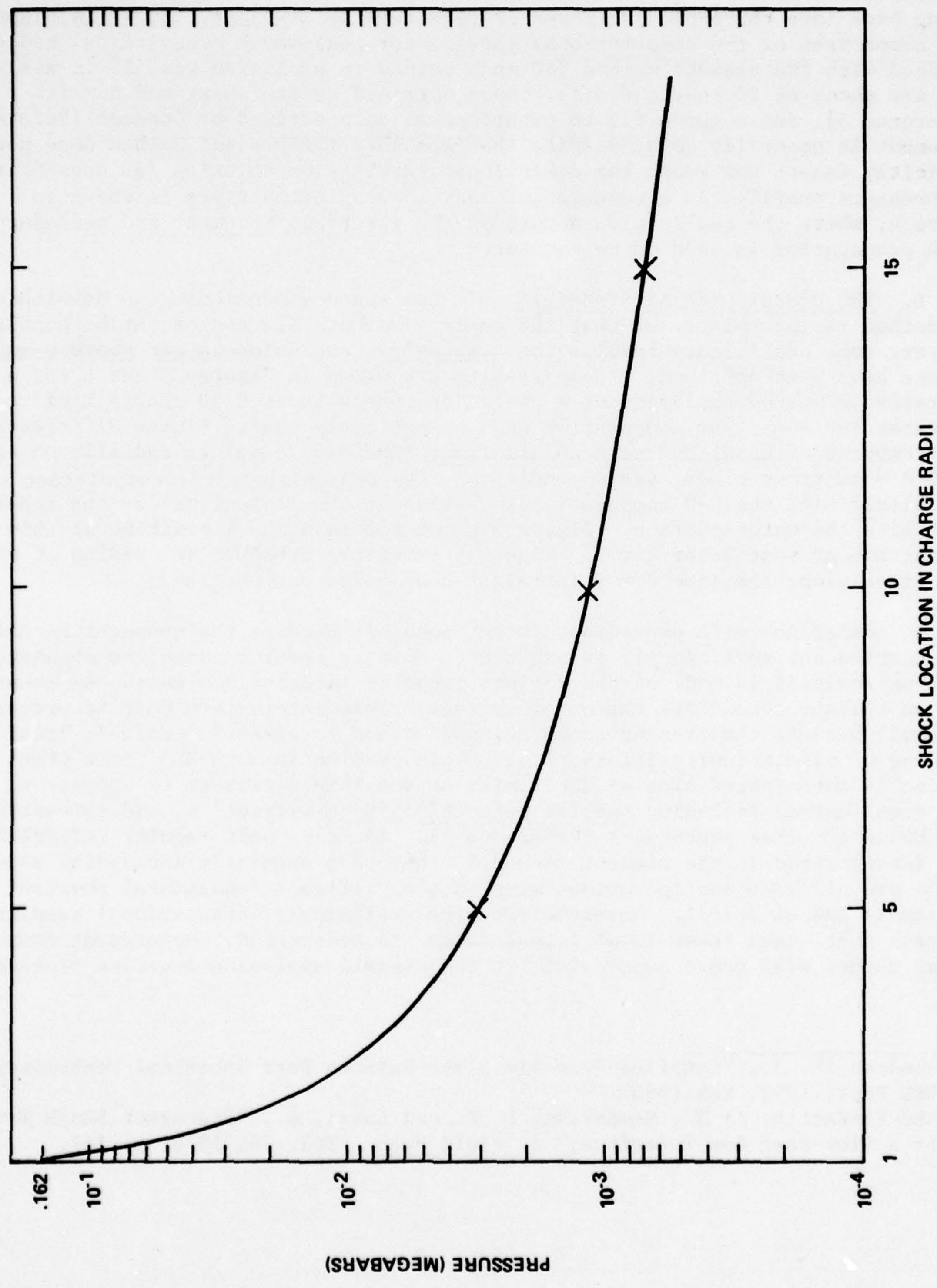

FIGURE 2 COMPUTED SHOCK PRESSURE VS. SHOCK LOCATION, PENTOLITE SPHERE CENTRALLY DETONATED IN WATER (X INDICATES STERNBERG/HURWITZ RESULT – OTHER VALUES EQUALLY CLOSE)

(ii) Spherical Explosion of Pentolite in $\gamma = 1.4$ Air. This problem is more difficult than the explosion in water case because the initial rarefaction moving back into the explosive gases is considerably stronger. Shown in Figure 3 is a comparison of the computational results for peak shock pressure vs. radius obtained with the present method (40 mesh points in explosive gas, 15 in air when main air shock at 20 charge radii), those obtained by Sternberg and Hurwitz [Reference 5], and a curve fit to experimental data derived by Goodman [Reference 6]. Agreement is generally good, despite the fact that the present method does not explicitly insert the known one dimensional rarefaction solution (as does Sternberg). The pressure profiles as a function of radius at selected times is shown in Figure 4, where the qualitative nature of the interface movement and secondary shock propagation is seen to be correct.

B. TWO DIMENSIONAL AXISYMMETRIC. In two space dimensions, the development of the method is incomplete, so that the entire EAAW problem cannot yet be handled. However, some preliminary results for a spherical explosion in air above a water surface have been obtained. These results are shown in Figures 5 and 6 for a centrally detonated explosion of a pentolite sphere located 30 charge radii above the water surface. The computation used an extremely coarse finite difference mesh composed of about 500 mesh points (approximately 25 points radially on each of 20 θ = constant lines; see Appendix A). The 2-D axisymmetric computation was initialized with the 1-D computational results at the instant before the spherical shock hits the water surface. Figure 5 shows the main shock position at this instant and at some later times. Figure 6 shows the pressure vs. radius at these same times along the line $\theta = 0$ (straight down below the charge).

No comparison with experiment is yet possible because the computation has not been carried out sufficiently far in time. Further results cannot be obtained until an analysis is made of the various types of interactions which can occur when an oblique shock hits the water surface. This interaction must be understood in detail because the present computational method requires an explicit local handling of discontinuity interactions. This problem is more difficult than originally anticipated because the family of possible interactions appears to be very complicated, including regular refraction, Mach refraction, and refraction with bound and free precursors [Reference 7]. (So far, only regular refraction has been incorporated in the present method.) Thus this seemingly incidental aspect of the overall EAAW configuration is in fact a difficult fundamental physical problem in and of itself. Nevertheless, the preliminary computational results indicate that, once these local interactions are understood, the present computational method will prove successful for the overall explosion dynamics problem.

---

6. Goodman, H. J., "Compiled Free-Air Blast Data on Bare Spherical Pentolite," BRL Rept. 1092, Feb 1960.
7. Abd-El-Fattah, A. M., Henderson, L. F., and Lozzi, A., "Precursor Shock Waves at a Slow-Fast Gas Interface," J. Fluid Mech., Vol. 76, 1976, p. 157.

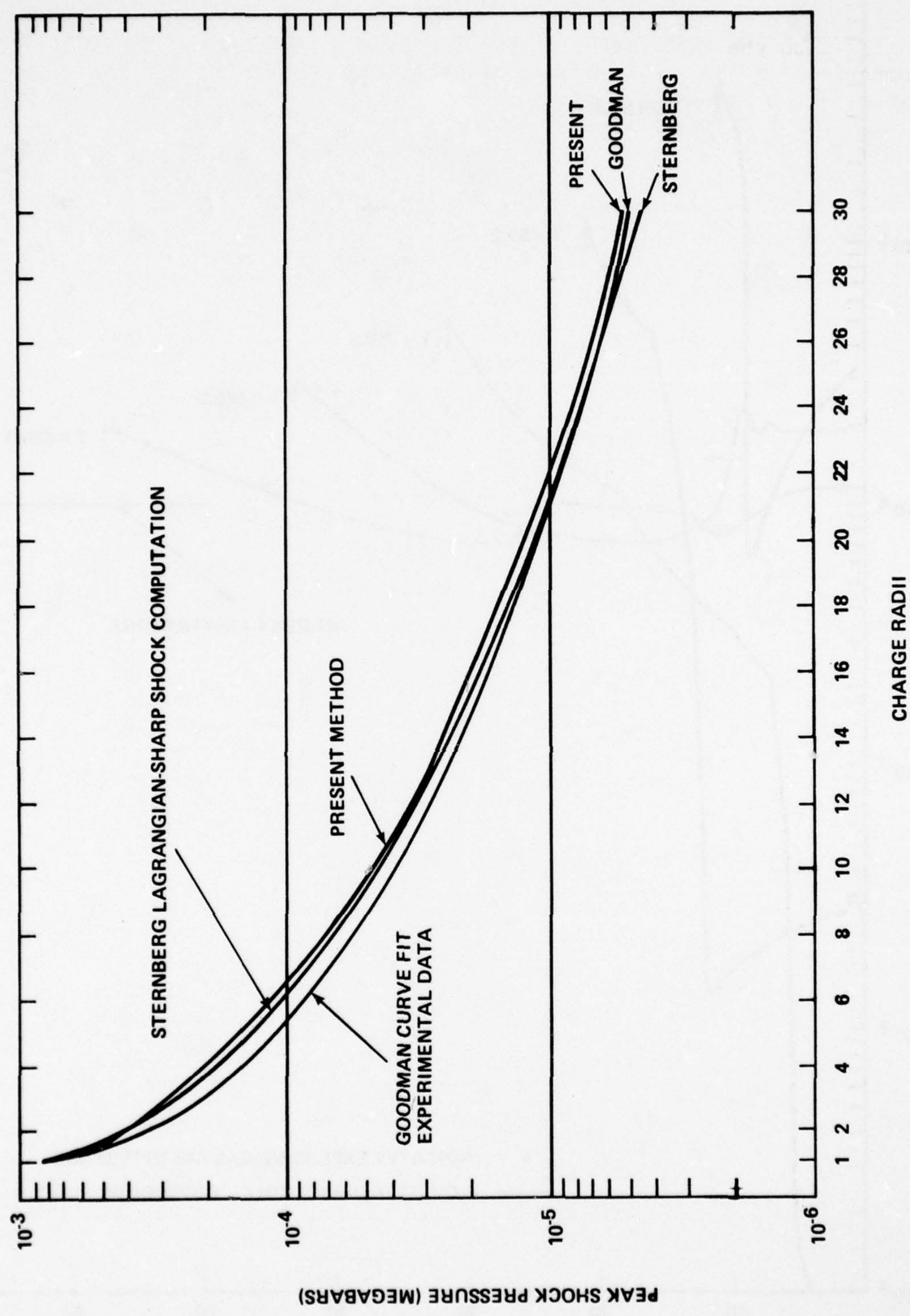

FIGURE 3 PEAK SHOCK PRESSURE VS. SHOCK LOCATION, PENTOLITE SPHERE CENTRALLY DETONATED IN γ = 1.4 AIR

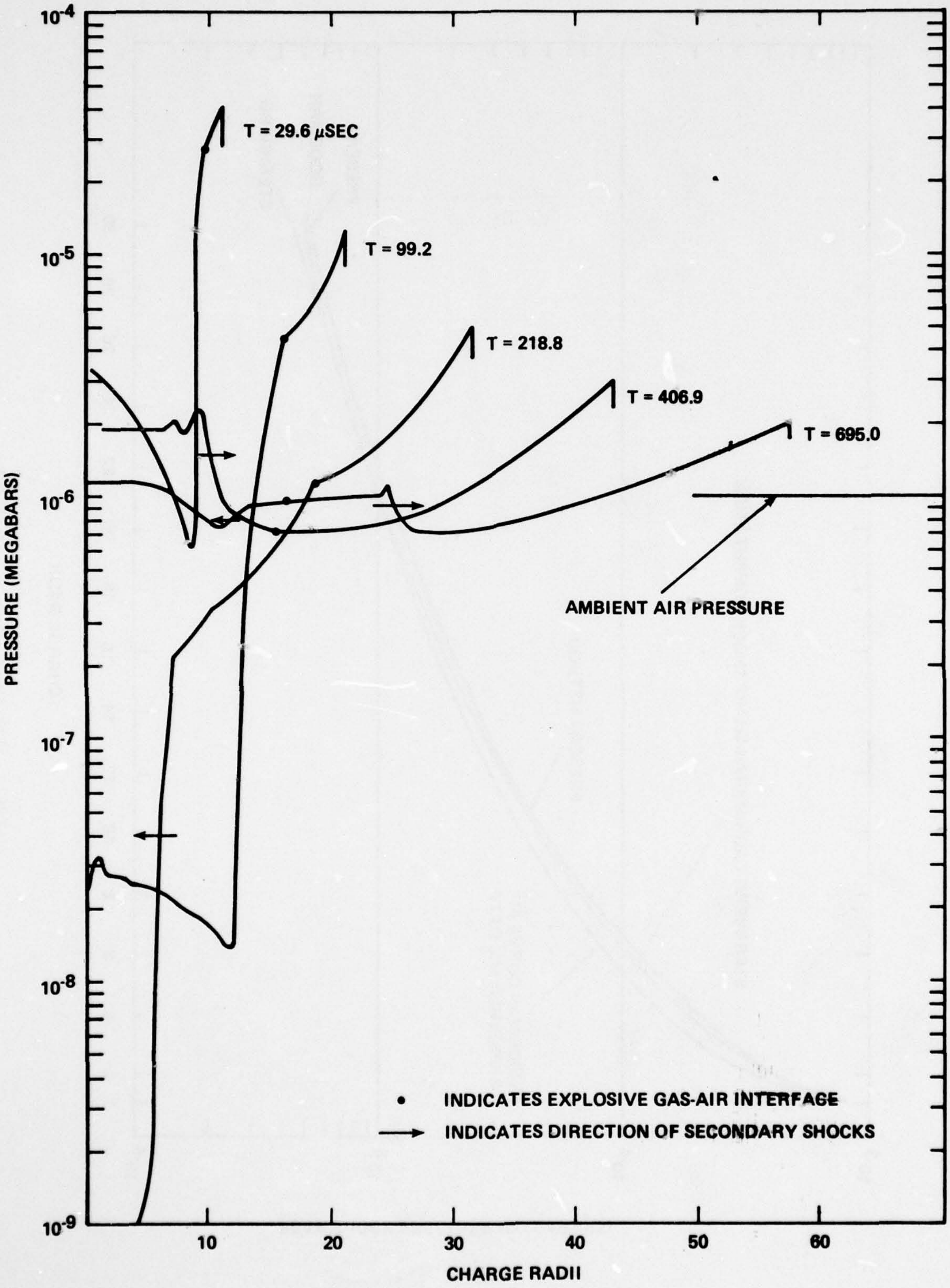

FIGURE 4 PRESSURE VS. RADIAL DISTANCE AT VARIOUS TIMES, PENTOLITE SPHERE CENTRALLY DETONATED IN $\gamma = 1.4$ AIR

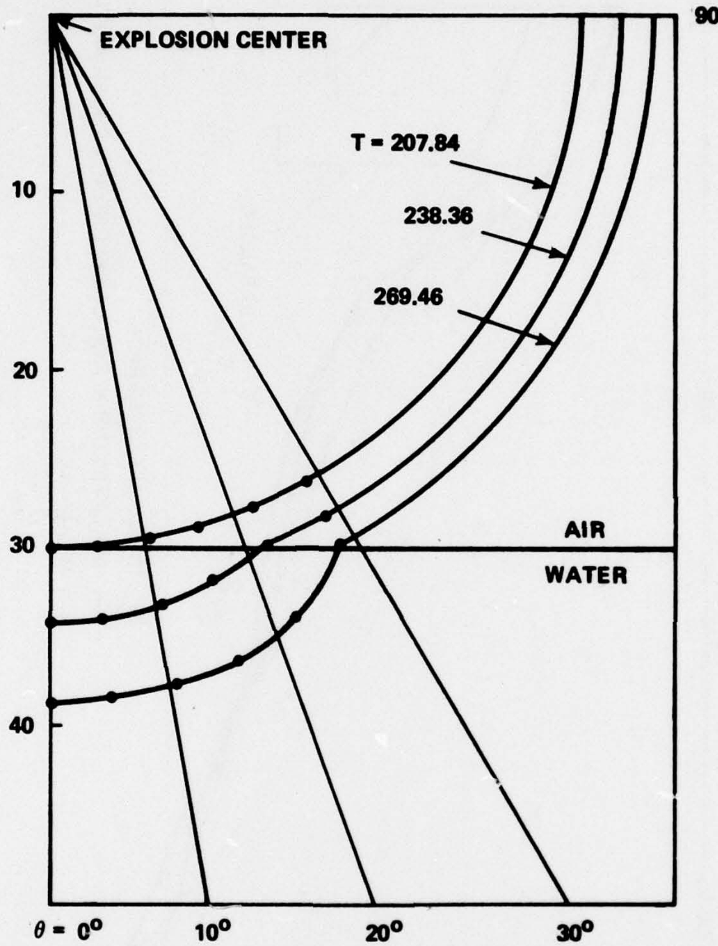

FIGURE 5 MAIN SHOCK LOCATION AT VARIOUS TIMES, PENTOLITE SPHERE CENTRALLY DETONATED IN AIR 30 CHARGE RADII ABOVE FLAT WATER SURFACE

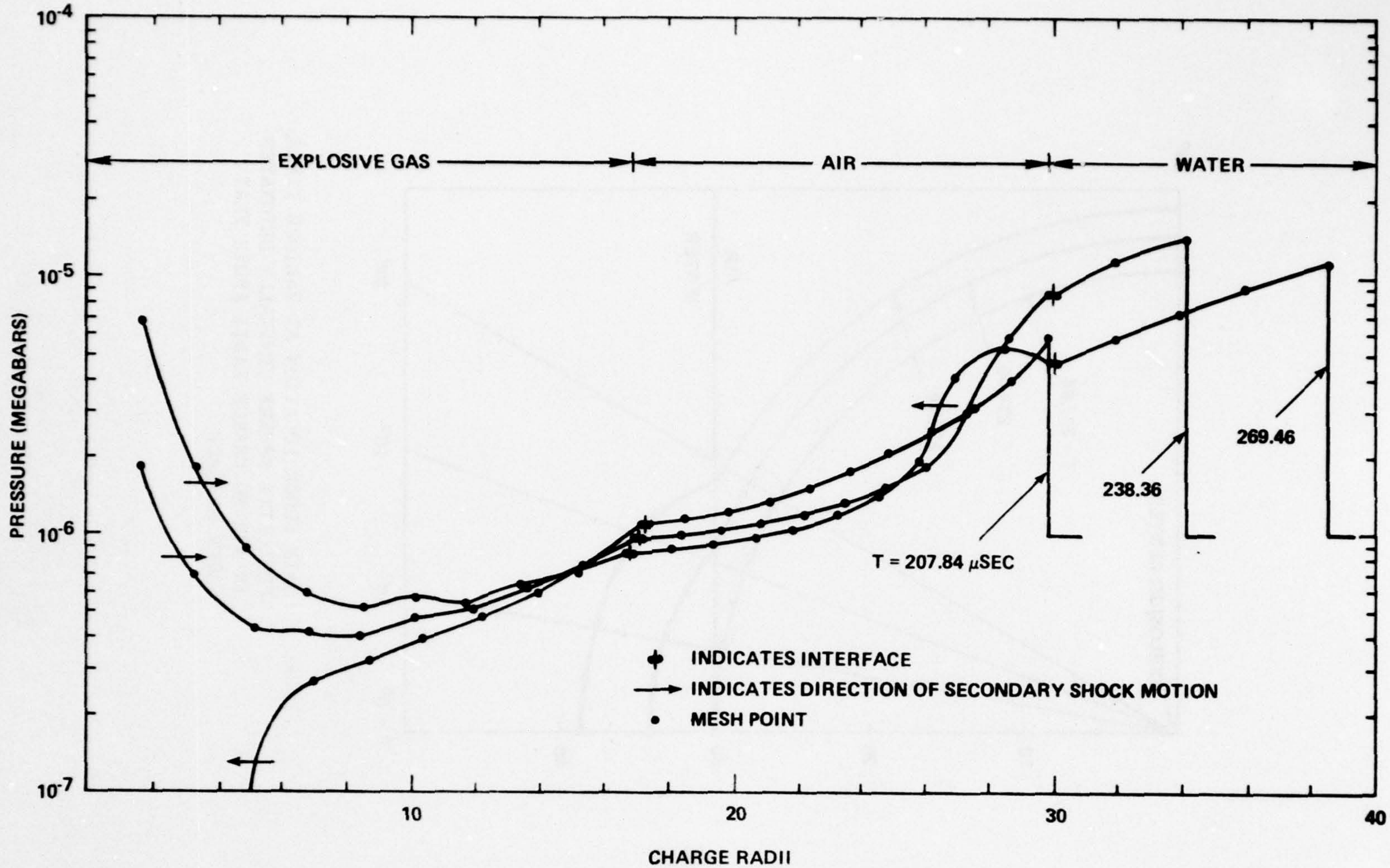

FIGURE 6 PRESSURE VS. RADIAL DISTANCE AT VARIOUS TIMES, STRAIGHT DOWN BELOW CHARGE ($\theta = 0$), PENTOLITE SPHERE CENTRALLY DETONATED IN AIR 30 CHARGE RADII ABOVE FLAT WATER SURFACE

APPENDIX A

DETAILED DESCRIPTION OF THE COMPUTATIONAL METHOD

This appendix contains an exposition of the basic mathematical and numerical techniques which underlie the sharp discontinuity tracking method, but does not give a detailed explanation of its implementation.

A1. GOVERNING EQUATIONS

The equations of inviscid unsteady flow are written in spherical coordinates r,θ,ϕ (Figure A-1) for an axisymmetric problem ($\partial/\partial\phi \to 0$, $r \geq 0$, $0 \leq \theta \leq \pi$) as the following system of weak conservation laws:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial r} + \frac{\partial G}{\partial \theta} + H = 0 \qquad \text{(A-1)}$$

where

$$U = r^2 \sin\theta \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{pmatrix} \qquad F = r^2 \sin\theta \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(\rho E + p) \end{pmatrix}$$

$$G = r\sin\theta \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(\rho E + p) \end{pmatrix} \qquad H = \begin{pmatrix} 0 \\ -(2p+\rho v^2) r\sin\theta \\ -r(p\cos\theta - \rho uv\sin\theta) \\ 0 \end{pmatrix} \qquad \text{(A-2)}$$

Here ρ is the density, u is the r-component of velocity, v is the θ-component of velocity, e is the specific internal energy, and $E = e + (u^2+v^2)/2$ is the total specific energy. The pressure p is given by an equation of state for each fluid (see References 5,8 for equations of state for pentolite, air, and water) in the form

$$p = p(\rho, e) \qquad \text{(A-3)}$$

8. Walker, W. A. and Sternberg, H. M., "The Chapman-Jouguet Isentrope and the Underwater Shock Wave Performance of Pentolite," Proceedings of the 4th Symposium (International) on Detonation, ACR-126, U.S. Gov't Printing Office, 1965, p. 27.

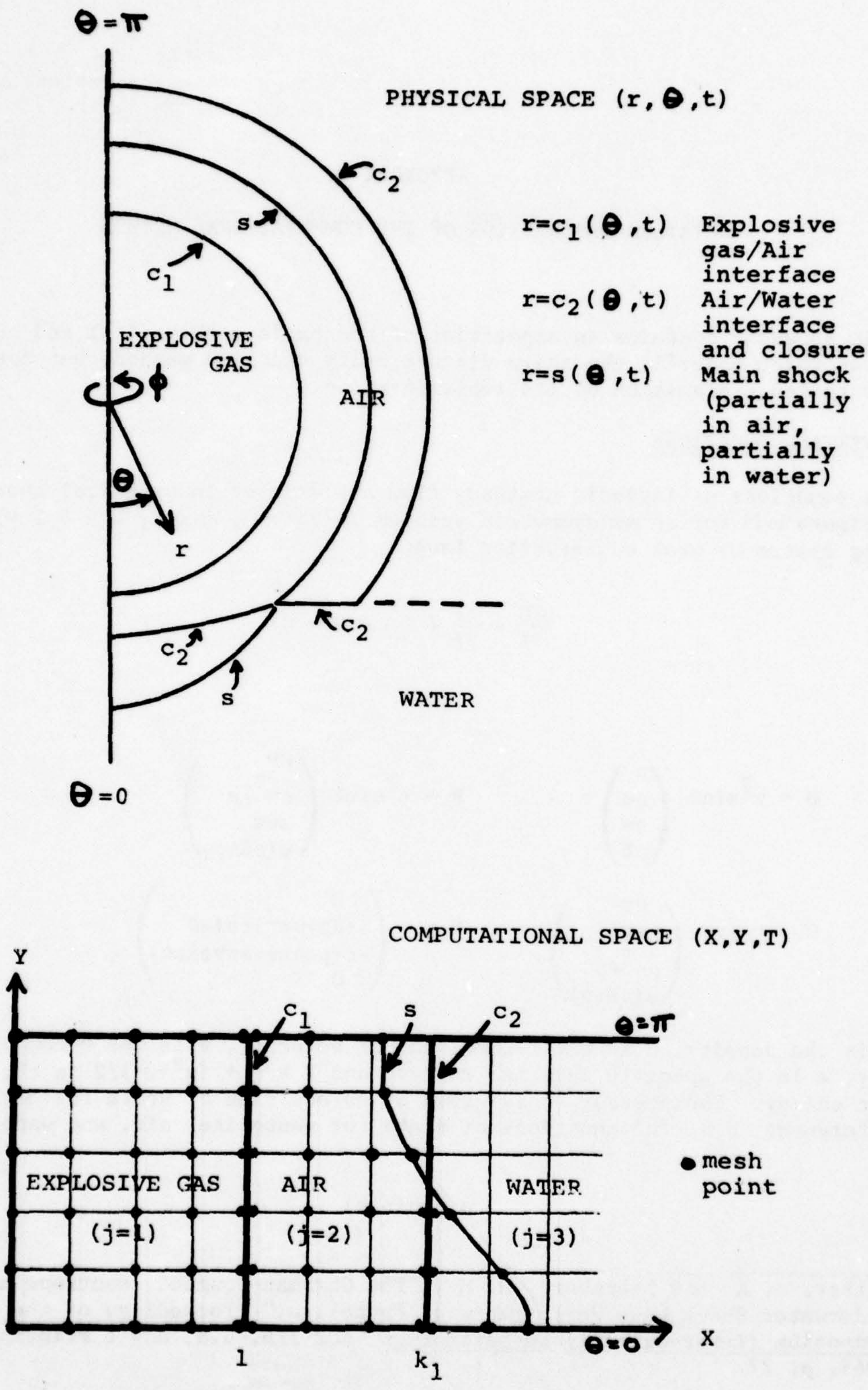

FIGURE A-1 PHYSICAL AND COMPUTATIONAL SPACE FOR AXISYMMETRIC PROBLEM OF SPHERICAL EXPLOSION ABOVE AN INITIALLY FLAT WATER SURFACE

A "main" shock wave is defined by the surface $r = s(\theta,t)$ and contact discontinuities are given as $r = c_i(\theta,t)$, $i = 1,2,\cdots I$. For the explosion in air above water, $I = 2$ and c_1 is the contact surface separating the explosive gas products from air, while c_2 is the air-water surface (plus an appropriate closure for large θ, see Figure A-1). The main shock is, in general, partially in air and partially in water. These major discontinuities s and c_i are unknowns which must be advanced in time by the solution procedure. "Secondary" shocks and contact discontinuities are allowed to be smeared out by the finite difference scheme used for interior mesh points, as discussed below.

It is noted that the choice of the form of equations system (A-1) eliminates the need to specify boundary conditions on $r = 0$ and on the symmetry boundaries $\theta = 0,\pi$ since the unknown U is identically zero there. This is consistent with the fact that by symmetry, $u = v = 0$ at $r = 0$ and $v = 0$ on $\theta = 0,\pi$. However, if it is desired to obtain a solution on $\theta = 0,\pi$, it is necessary to derive another set of equations which hold only on $\theta = 0$ and $\theta = \pi$; this is easily done by dividing (A-1) by $\sin\theta$ and using L'Hopital's rule to evaluate the limits $\theta \to 0,\pi$.

A2. COMPUTATIONAL PROCEDURE

The computational field is viewed as being composed of regions of relatively smooth flow which are separated from each other by explicit discontinuities--either shocks or contact discontinuities. It is convenient to employ a time dependent transformation which always maps the contact discontinuities c_i, which are single-valued, piecewise smooth curves in physical space, into coordinate lines in computational space (Figure A-1). It will be seen that, for the explosion in air above water (EAAW), this has the advantage of preserving computational resolution in the air region $c_1 \leq r \leq c_2$, even if $c_2 - c_1$ becomes small.

The transformation from physical to computational space is given generally as

$$\begin{aligned} X &= X(r,\theta,t) \\ Y &= Y(\theta) \\ T &= t \end{aligned} \tag{A-4}$$

and the governing partial differential equations (A-1) are expressed in the transformed computational space (X,Y,T) as

$$\frac{\partial U}{\partial T} + \frac{\partial \tilde{F}}{\partial X} + \frac{\partial \tilde{G}}{\partial Y} + \tilde{H} = 0 \tag{A-5}$$

where

$$\begin{aligned} \tilde{F} &= X_t U + X_r F + X_\theta G \\ \tilde{G} &= Y_\theta G \\ \tilde{H} &= H - \frac{\partial X_t}{\partial X} U - \frac{\partial X_r}{\partial X} F - \left(\frac{\partial X_\theta}{\partial X} + \frac{\partial Y_\theta}{\partial Y}\right) G \end{aligned} \tag{A-6}$$

Once a specific choice of transformation (A-4) is made, the quantities $X_t, X_r, X_\theta, Y_\theta$, and their partial derivatives are given explicitly in terms of $s(\theta,t)$, $c_i(\theta,t)$, and their partial derivatives.

For the EAAW problem, convenient choices of the transformation X are:

gas region: $0 \leq r \leq c_1(\theta,t)$

$$X = \frac{r}{c_1(\theta,t)}$$

air region: $c_1(\theta,t) \leq r \leq c_2(\theta,t)$

$$X = 1 + (k_1-1)\left[\frac{r-c_1(\theta,t)}{c_2(\theta,t)-c_1(\theta,t)}\right] \tag{A-7}$$

water region: $c_2(\theta,t) \leq r$

$$X = k_1+k_2[r-c_2(\theta,t)]$$

so that $r = c_1(\theta,t)$ is mapped into $X = 1$, and $r = c_2(\theta,t)$ is mapped into $X = k_1$. Then for a given number of mesh points in the X-direction in the explosive gas region, the choices of k_1 and k_2 give the relative computational resolution in the air and water regions respectively. A convenient choice of the transformation Y is (in inverted form)

$$\theta = \pi\left(\frac{\omega^Y - 1}{\omega - 1}\right)$$

where ω is a parameter which gives graded resolution in physical space with finest resolution near $\theta = 0$ if $\omega > 1$.

A mesh function $U^k_{m,n,j}$ is defined on the uniform computational mesh

$$\text{for } j=1,2,3 \quad \left|\begin{array}{ll} X = m\Delta X & m = 0,1,2,\cdots,M(j) \\ Y = n\Delta Y & n = 0,1,2,\cdots,N \\ T = T_o+k\Delta T & k = 0,1,2,\cdots \end{array}\right.$$

where $m(1)\Delta X = 1$, $m(2)\Delta X = k_1 - 1$, $N\Delta Y = 1$, and $j=1,2,3$ for the regions of explosive gas, air, and water respectively (Figure A-1). The main shock defined by $r = s(\theta,t)$ in physical space "floats" through the uniform mesh and is represented by special mesh points which are located on Y = constant lines.

It is assumed that initial data (see, e.g., Reference 8) is given $T = T_o$ for $\rho,u,v,e,p,c_1(\theta,t_o)$ and $s(\theta,t_o)$ on the spatial mesh defined above. In order to advance the solution to $T_o + \Delta T$, procedures must be given for

(i) "interior" points ($1 \leq m \leq M(j) - 1$, $1 \leq n \leq N - 1$)

(ii) points on the symmetry boundaries $\theta = 0,\pi$ ($n = 0,N$)

(iii) shock points

(iv) contact discontinuity points ($j = 1$, $m = M(1)$; $j = 2$, $m = 1$ and $m = M(2)$; $j = 3$, $m = 1$)

(v) interactions between a shock and a contact discontinuity

The solution at all points is advanced in time using finite difference predictor-corrector methods. For the interior points (i), the equations (A-5) are discretized and standard MacCormack [Reference 9] schemes (in this case, predictor forward differencing and corrector backward differencing in both X and Y) are used to advance the conservation vector U. The primary flow variables are easily recovered from the definition of U and the equations of state. Points on the symmetry planes (ii) are advanced in the same way, only the governing equations must be modified (as described above) before discretization. The procedures for advancing the remaining points, namely those at the shock, the contact discontinuities, and the points of discontinuity interaction, are described later.

The MacCormack finite difference scheme was chosen for its second order accuracy and its good "shock-capturing" properties (ability to reasonably smear out a shock over several mesh points), but any other predictor-corrector method could be used. For very strong shocks, such as the secondary shock which implodes on the origin in a spherical explosion, it is necessary to implement a computational "filter" (similar to that in Reference 10) to limit shock steepening. Any other shock capturing "improvement" may also be included.

Computational stability demands that ΔT be suitably restricted. A necessary (but not sufficient [Reference 11]) criterion can be derived using a geometric argument which requires that the domain of dependence of the "linearized" differential equations be contained in the domain of dependence of the finite difference equations. When this criterion is used with a multiplicative safety factor of .9, no instability is observed in actual computation.

A3. ADVANCING THE MAIN SHOCK AND CONTACT DISCONTINUITIES

A crucial requirement of the present computational method is to provide an appropriate numerical treatment of the explicit surfaces which represent shocks or contact discontinuities. The known physical boundary conditions, namely the Rankine-Hugoniot jump conditions and the equality of tangential velocity across a shock, and the equality of pressure and normal velocity across a contact discontinuity, must hold exactly. However, these boundary conditions alone are not sufficient to provide equations for advancing the surface in time, but must be considered along with appropriate information obtained from the governing PDE system (A-1). From the theory of characteristics for hyperbolic systems of PDE's, one can derive characteristic compatability conditions (see Reference 12) which are associated with certain bicharacteristic directions. Admissable characteristic

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9. MacCormack, R. W., "The Effect of Viscosity in Hypervelocity Impact Cratering," AIAA Paper No. 69-354, 1969.
10. Harten, A., "The Artificial Compression Method for Computation of Shocks and Contact Discontinuities. I. Single Conservation Laws," Comm. Pure. Appl. Math, Vol. XXX, 1977, p. 611.
11. Turkel, E., "Phase Error and Stability of Second Order Methods for Hyperbolic Problems I," Journal of Computational Physics, Vol. 15, June 1974, p. 226.
12. Courant, R. and Hilbert, D., Methods of Mathematical Physics, Vol. II, Interscience, N.Y., 1962.

relations, that is, those associated with directions pointing away from the surface in the negative time direction, effectively "tell" the surface what is happening in the surrounding fluid. In the manner introduced by Kentzer (Reference 13) and used by Solomon et al. (References 1, 2), it is possible to combine the physical boundary conditions with the correct characteristic compatability relations to obtain a system of PDE's which hold only on the surface. A finite difference approximation of these equations then provides the algorithm for advancing the surface, and the flow properties on either side, in time.

(i) CONTACT DISCONTINUITY. A contact discontinuity (c.d.) $r = c(\theta,t)$ is a material surface for the fluids on either side of the discontinuity. Hence

$$c_t - u + \frac{c_\theta}{c} v = 0 \tag{A-8}$$

holds at a c.d. (subscripts t,θ indicate partial derivatives). There are three admissable characteristic compatability relations which hold on each side (left and right) of the surface. Two relations correspond to a streamline and one to the Mach conoid. These compatability relations are of the form

$$\frac{\partial p}{\partial T} - A_1 \frac{\partial \rho}{\partial T} = R_1 \tag{A-9}$$

$$\frac{\partial}{\partial T} (D_c q_{tang}) - u \frac{\partial}{\partial T}\left(\frac{c_\theta}{c}\right) = R_2 \tag{A-10}$$

$$A_2 \frac{\partial p}{\partial T} + A_3 \left[\frac{\partial c_t}{\partial T} + v \frac{\partial}{\partial T}\left(\frac{c_\theta}{c}\right)\right] = R_3 \tag{A-11}$$

It is emphasized that (A-9)-(A-11) hold on each side of the surface, and hence represent six equations. R_1 and R_2 contain derivatives interior to the surface (Y-derivatives) and undifferentiated quantities evaluated at the surface, while R_3 contains additionally X-derivatives. A_1, A_2, and A_3 contain only undifferentiated quantities, and $D_c^2 = 1 + \left(\frac{c_\theta}{c}\right)^2$. The pressure p and the normal velocity $q_{norm} = \frac{c_t}{D_c}$ are constant across the c.d., while the density ρ, energy e, and tangential velocity q_{tang} can sustain jumps.

In addition to the characteristic compatability relations we have the equation

$$\frac{\partial}{\partial T}\left(\frac{c_\theta}{c}\right) = \frac{Y_\theta}{c}\left[\frac{\partial c_t}{\partial Y} - \frac{c_t}{c}\frac{\partial c}{\partial Y}\right] \tag{A-12}$$

13. Kentzer, C. P., "Discretization of Boundary Conditions on Moving Discontinuities," Lecture Notes in Physics, Vol. 8, Springer-Verlag, 1971, p. 108.

which expresses, through the chain rule, the equality of cross partials $\frac{\partial c_\theta}{\partial t} = \frac{\partial c_t}{\partial \theta}$. Also

$$\frac{\partial p}{\partial T} = K_1 \frac{\partial \rho}{\partial T} + K_2 \frac{\partial e}{\partial T} \tag{A-13}$$

holds on each side, where $K_1 = \left(\frac{\partial p}{\partial \rho}\right)_e$ and $K_2 = \left(\frac{\partial p}{\partial e}\right)_\rho$ are given by the appropriate equations of state. A procedure is now clear for advancing the c.d., since equations (A-9)-(A-13) provide nine equations in the nine unknowns which are (the time derivatives of) $c_t, c_\theta, p, [\rho, e, q_{tang}]_{Left}, [\rho, e, q_{tang}]_{Right}$.

(ii) <u>SHOCK</u>. A shock $r = s(\theta,t)$ is a surface across which the Rankine-Hugoniot jump conditions hold, namely

$$\rho Q_{norm} = \text{constant} \tag{A-14}$$

$$p + \rho Q^2_{norm} = \text{constant} \tag{A-15}$$

$$e + p/\rho + Q^2_{norm/2} = \text{constant} \tag{A-16}$$

where q_{norm} is the velocity normal to the shock in (r,θ) coordinates, $D_s = 1 + \left(\frac{s_\theta}{s}\right)^2$ and $Q_{norm} = q_{norm} - \frac{s_t}{D_s}$ is the relative velocity normal to the moving shock surface. Additionally, the tangential velocity is unchanged across a shock,

$$q_{tang} = \text{constant} \tag{A-17}$$

Only shocks moving into undisturbed fluid are considered here. For this case, there is only one admissible characteristic compatability relation, and it corresponds to a Mach conoid on the disturbed (high pressure) side of the shock. The compatability condition is of the form

$$\frac{\partial p}{\partial T} + A_4 \frac{\partial q_{norm}}{\partial T} = R_4 \tag{A-18}$$

where R_4 contains derivatives in the X-direction, derivatives interior to the shock, and undifferentiated quantities. Differentiating (A-14)-(A-16) with respect to T and solving for $\frac{\partial p}{\partial T}$ and $\frac{\partial q_{norm}}{\partial T}$, it is possible to rewrite (A-18) as

$$A_5 \left[\frac{\partial s_t}{\partial T} - A_6 \frac{\partial}{\partial T}\left(\frac{s_\theta}{s}\right)\right] = R_4 \tag{A-19}$$

where A_5 and A_6 contain only undifferentiated quantities. The equality of cross partials, expressed through the chain rule, is of the form

$$\frac{\partial}{\partial T}\left(\frac{s_\theta}{s}\right) = R_5 \qquad \text{(A-20)}$$

so that (A-19) and (A-20) provide equations for advancing s_θ and s_t. It is then easy to get the advanced value of q_{norm} and use the Hugoniot conditions (A-14)-(A-16) to solve for all properties behind the shock.

(iii) COMMENTS. For either a shock or a c.d., we have a system of PDE's for advancing (in time) the surface and the flow variables on either side. These equations are implemented with a predictor-corrector finite difference method. Spatial differencing internal to the surface is handled in the usual predictor-forward, corrector-backward way. However, differencing in the X-direction requires special treatment since no differences can be taken across the discontinuity. Thus at the left side of discontinuities the differencing is always backward (both predictor and corrector), whereas on the right side the differencing is always forward. This procedure is only first order accurate, but it is possible (Reference 14) to add a correction term to achieve overall second order accuracy.

At the shock, finite differences are taken on a non-uniform mesh, but again it is possible to secure second order accuracy by adding a correction term. Additionally, since the shock is moving into a previously undisturbed fluid where there are no mesh points, it is necessary to insert new mesh points behind the advancing shock. This is done by quadratic interpolation of the conservation vector U using the known primary flow variables at the shock and the values of U at the mesh points along Y = constant lines behind the shock.

A4. INTERACTIONS

Since the sharp discontinuity tracking method treats physically important discontinuities as explicit surfaces, it is necessary to analyze the situation which occurs when two such discontinuities interact. Considered here is the case of an air shock hitting the air-water surface obliquely. It appears that the qualitative nature of the resulting physical phenomena depends upon the incident shock strength and the angle at which the discontinuities meet [Reference 7]. For sufficiently strong shocks and sufficiently small incidence angles α, a "regular refraction" solution exists as shown in Figure A-2. In a coordinate system moving along the surface with point A, the flow is pseudo-steady. Assuming locally constant states near A and locally plane discontinuities, the problem is reduced to an algebraic one of finding the twelve unknowns (ρ,u,v,e,p in regions 3 and 4, β,γ) which satisfy twelve nonlinear equations (Rankine-Hugoniot jump conditions and constancy of tangential velocity across each of R and W, state equations in regions 3 and 4, contact discontinuity conditions across the disturbed water surface).

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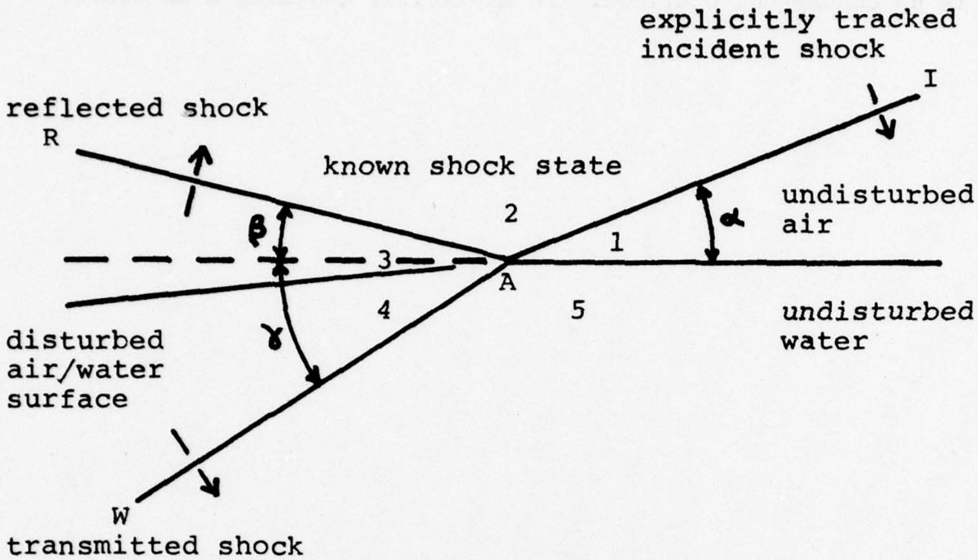

FIGURE A-2 REGULAR REFRACTION OF AIR SHOCK AT AIR/WATER INTERFACE

This locally exact solution gives the necessary information to track the transmitted water shock W and the disturbed air-water interface. At present the reflected shock is allowed to be smeared out by the MacCormack finite differencing, but there is no conceptual difficulty in explicitly tracking R as well.

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